C. THEMATIC BASIS FOR GROUP EFFORT

The last decade has seen immense progress in information technology, new materials, and biotechnology balanced against increasing stress to our planet from burgeoning human population and accelerating modification of our physical and biological environment. Will the new century be one of technological triumph, environmental disaster, or will we follow other paths not yet envisioned? Addressing such questions must meld science, technology, and the social and humanistic disciplines. We need integrative, rather than reductionist, thinking. Tractable solutions to these environmental problems require the whole spectrum of human intellectual activity, including physics, chemistry, biology, engineering, economics, sociology, and policy. Training a new generation of broadly educated and flexible scientists and engineers to deal with complex problems in changing times is a critical societal need. Yet, with this recognition of need, we face a vacuum of implementation. Most graduate education is organized along classical departmental and disciplinary lines, and students are often trained to do just one thing, hopefully well. We know of no significant doctoral programs which embody such integrative training in any area of environmental studies, particularly in the general focus area of this proposal, which we could call environmental materials science.

The ambition of this IGERT proposal is to combine the research and teaching interests of fourteen investigators in seven different departments ranging from physics to veterinary medicine in four different colleges around the unifying theme of NEAT (Nanomaterials in the Environment, Agriculture, and Technology). We use this focus to produce an integrative effort in environmental materials science in the broadest sense. This program at UC Davis represents a unique opportunity in a fertile intellectual environment. UC Davis combines historically strong roots in agriculture and environmental sciences with rapidly growing programs of excellence representing new directions in biology, the physical sciences, and engineering.

Nanomaterials are small particles having large surface areas and enhanced chemical and biologically reactivity, which figure prominently in fundamental science, technology, and transport of adsorbed pollutants and nutrients in the hydrosphere, atmosphere, and biosphere. We will educate students in the fundamental physical science needed to identify, characterize, and understand nanomaterials, in the constellation of environmental, geological, atmospheric and biological issues related to small particles, and in the regulatory and societal issues that arise or are impacted by such research. The faculty, students, and dissertation projects will be shared among the diverse departments and disciplines. We plan to develop common courses in basic science and laboratory and field techniques, a course on the ethics and communication skills requisite for such integrative research, and an ongoing seminar series to create a shared knowledge base. Students will be mentored both by a maximally diverse dissertation committee with ex officio members from laboratories and industry as well as
by senior students within the program. Coursework will be complemented by fieldwork and internships involving specific environmental nanomaterial occurrences, applications, and problems. Students will participate in the full range of IGERT based activities, from roundtable discussions about scientific, technical, and societal issues, to the actual structure and management of the group. The Ph.D.’s from this program will be well poised to embark on careers in basic research, environmental management and remediation, health sciences, and public policy and legislative development.

Modern materials science stresses low temperature ceramic processing (sol gel, chimie deuce, self assembly, templating using organic-inorganic interactions). Advances are being made because modern synthetic, computational, and characterization tools are now available, and quantitative fundamental science can be done. Modern earth science (mineralogy, mineral physics) is beginning to apply similar sophisticated analysis to the nanophases encountered in nature - clays, zeolites, and oxyhydroxides. Catalysts are largely nanophases, as are paints, coatings, and fibers. Cements are notorious for their poorly crystalline constituents and cement science is starting to deal with fundamental issues. The containment or dispersal of potential pollutants, including nuclear waste, is often mediated by nanomaterials. Soil science and agriculture fundamentally encounter the same materials and phenomena, understanding of which is crucial to rational development of agricultural technology. Nanoparticles in the atmosphere arise from both geological and human processes; dust particles carried over the globe affect health, act as nucleation sites for cloud formation and rain, and affect climate. Zeolites, clays, hydrated aluminosilicates, and iron and manganese oxides and oxyhydroxides, in myriad forms, modifications, and degrees of crystallinity, form the inorganic components of soils. Biological processes almost invariably take place at the nanoscale, across membranes and at interfaces. Transport and retention of inorganic elements in the environment is mediated by nanophases. The role of biological processes in changing the inorganic surface of this planet is just being recognized. Many bacteria use inorganic oxidation-reduction cycles as energy sources.

The fundamental phenomena associated with nanoscale materials are very similar, whether the particle in question is iron oxide in soil, a coated particle for magnetic recording, a zeolite added to animal feed, or a particle of carbonaceous or silica dust emitted from a smokestack. Addressing these questions requires theoretical and experimental physics, chemistry, and materials science. UC Davis has a number of strong groups working in this fundamental area: Navrotsky in thermodynamics, Kauzlarich, Patten, Kennedy, and Risbud in synthesis and characterization, Gates in catalysis, Casey in surface characterization and NMR studies of structure and reactivity, and Pickett and Cox in the theory and modeling of structure, spectra, and reactivity. This science forms the backbone of all applications.

Transport of nanoparticles in the environment occurs in both water and air: the former by both dissolution and by colloidal particles and their adsorbed pollutants (or nutrients), the latter as dust, aerosols, and adsorbed contaminants. Much contaminant movement (organic chemicals in a waste plume, radionuclides in a nuclear waste site, agricultural chemicals in dust over farmland) occurs by transport of nanoparticles and colloids. To understand such transport, one must first characterize the nanoparticles and their source. One must then understand their physical transport through fluid flow or air movement, identify changes in the chemistry and morphology of the particles as they move. Finally one must identify their ultimate fate, either dissolution or agglomeration into larger, no longer easily transported, forms. To unravel these transport processes one must understand the basic physics and chemistry and the hydrology and
meteorology pertinent to transport. Anastasio, Kennedy, and Casey provide this linkage. The unique feature here will be to train students to be competent in both atomistic and transport aspects. An additional benefit may be to use chemical probes and characterization tools to better identify the sources and sinks of particles.

Nanoparticles interact strongly with the biosphere. One such interaction is by transformation of nanoparticles by microorganisms. Bacteria utilize the variable valence ions in inorganic nanoparticles (e.g., Mn and Fe) as energy sources in anaerobic oxidation-reduction reactions. Scow, Montañez, and Navrotsky can address issues of energetics and microbial transformations. Nanoparticles which penetrate the lungs are toxic. Yet the fundamental mechanisms of particle-host interaction remain unclear. We will team materials scientists who can produce and characterize nanoparticles (Risbud, Kauzlarich, and Kennedy) with toxicologists who can study their biological effects (Pinkerton). Here there is a tremendous challenge in education, since the two groups typically speak very different scientific jargon and know little of each other’s fields. Training students to be cognizant of both the biological and the materials aspects is a major goal of this IGERT.

Finally, knowledge of the sources, sinks, and transformations of nanoparticles enables one to identify the origins of contamination and to rationally consider remediation schemes. Such knowledge will help our society choose among various options for pollution abatement, avoid unnecessary and expensive remediation schemes which have no basis in scientific knowledge, and implement regulatory policies based on knowledge rather than ignorance. There needs to be a strong connection between particles and policy. This is explored by Niemeier and others with an emphasis on automotive pollution. Training students to be familiar with both the scientific issues and the policy and regulatory environment is another goal of this IGERT. The major research effort described below is thus organized into our thrusts: (1) the basic science and technology of nanoparticles, (2) the transport and transformation of nanoparticles in the environment, (3) the interaction of nanoparticles with the biosphere, and (4) nano to macro - from particles to policy.